

# New Inequalities in Equilibrium Statistical Mechanics

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## Abstract:

Recently, new thermodynamic inequalities have been obtained, which set bounds on the quadratic fluctuations of intensive observables of statistical mechanical systems in terms of the Bogoliubov - Duhamel inner product and some thermal average values. It was shown that several well-known inequalities in equilibrium statistical mechanics emerge as special cases of these results. On the basis of the spectral representation, lower and upper bounds on the one-sided fidelity susceptibility were derived in analogous terms. Here, these results are reviewed and presented in a unified manner. In addition, the spectral representation of the symmetric two-sided fidelity susceptibility is derived, and it is shown to coincide with the one-sided case. Therefore, both definitions imply the same lower and upper bounds on the fidelity susceptibility.

## I. INTRODUCTION

A number of important results on the role of critical fluctuations in systems with broken symmetries have been obtained in the past by using famous inequalities due to Bogoliubov, Mermin-Wagner, Griffiths, among others, see, e.g. [1–4]. A remarkable property of this approach is that the results obtained are exact and cannot be inferred from any perturbation theory. The benefits of having exact statements about systems with strongly interacting particles are difficult to overestimate.

The article is structured as follows. We begin by introducing notations and basic definitions of the models under consideration. In Section II, we review the recently obtained inequalities, in which the central role is played by the Bogoliubov - Duhamel inner product. In Section III we give the definitions of fidelity and its second derivatives: the one-sided and

symmetric two-sided fidelity susceptibilities. The new results concerning the derivation of a spectral representation for the symmetric two-sided fidelity susceptibilities are presented in Section IV. Since it turns out that the two spectral representations are the same, we note that both definitions imply the same lower and upper bounds, see Section V. The paper closes with some concluding remarks in Section VI.

We shall consider families of Hamiltonians depending on auxiliary external fields  $\nu$  and  $\nu^\star$  conjugate to the intensive operators  $A^\dagger$  and  $A$ , respectively,

$$\mathcal{H}(\nu) \equiv \mathcal{H} - |\Lambda|(\nu A^\dagger + \nu^\star A). \quad (1)$$

The quantum statistical mechanical models are defined initially in a finite region  $\Lambda$  of the  $d$ -dimensional Euclidean space  $R^d$  or the  $d$ -dimensional integer lattice  $Z^d$ . By  $|\Lambda|$  we denote the volume of  $\Lambda$  in the former case, or the number of lattice sites in the latter case.

The Hamiltonian  $\mathcal{H}(\nu)$  is defined as a self-adjoint operator in a separable Hilbert space  $\mathbf{H}$ , and the corresponding free energy density  $f_\Lambda[\mathcal{H}(\nu)]$  is assumed to exist. For the sake of simplicity, we do not explicitly distinguish between a Hamiltonian  $\mathcal{H}(\nu)$ , describing a system with fixed number of particles  $N$  in  $\Lambda$ , and the statistical operator  $\mathcal{H}(\nu) - \mu\mathcal{N}$  in the grand canonical ensemble, where  $\mu$  is the chemical potential and  $\mathcal{N}$  is the particle number operator. The density of the corresponding thermodynamic potential is given by

$$f_\Lambda[\mathcal{H}(\nu)] = -(\beta|\Lambda|)^{-1} \ln Z_\Lambda[\mathcal{H}(\nu)], \quad (2)$$

where  $Z[\mathcal{H}(\nu)] := \text{Tr} e^{-\beta\mathcal{H}(\nu)}$  is the partition function. Average values in the Gibbs ensemble with the Hamiltonian  $\mathcal{H}(\nu)$  are defined as

$$\langle \cdots \rangle_{\mathcal{H}(\nu)} \equiv \text{Tr}(e^{-\beta\mathcal{H}(\nu)} \cdots) / Z_\Lambda[\mathcal{H}(\nu)]. \quad (3)$$

In the theory of phase transitions a key role play the following quantities: the quadratic fluctuations

$$\langle \delta A \delta A^\dagger \rangle_{\mathcal{H}(\nu)}, \quad \delta A \equiv A - \langle A \rangle_{\mathcal{H}(\nu)}, \quad (4)$$

and the second derivative of the free energy density with respect to external fields  $\nu$ ,  $\nu^\star$ , i.e., the isothermal susceptibility

$$\chi_\Lambda(\nu) = -\frac{\partial^2 f_\Lambda[\mathcal{H}(\nu)]}{\partial \nu^\star \partial \nu}. \quad (5)$$

In what follows we will focus on the problem of relating (4) and (5) to other quantities that appear as indicators of phase transitions. Much work have been done on this issue in

the context of quantum information theory (see, e.g., [5, 6] and references therein). As a result, the knowledge obtained so far shows that techniques borrowed from the quantum information theory are likely to be useful in studying the phenomenon of phase transitions.

First of all we make use of the important relationship between (5) and the Bogoliubov - Duhamel inner product, defined as

$$(A; B)_{\mathcal{H}} \equiv (Z[\mathcal{H}])^{-1} \int_0^1 d\tau \operatorname{Tr} [e^{-\beta(1-\tau)\mathcal{H}} A^\dagger e^{-\beta\tau\mathcal{H}} B], \quad (6)$$

namely,

$$-\frac{1}{\beta|\Lambda|} \frac{\partial^2 f_\Lambda[\mathcal{H}(\nu)]}{\partial\nu^* \partial\nu} = (\delta A; \delta A). \quad (7)$$

This object has been introduced and discussed by a number of authors (see [2, 7] and references therein), which noted that it is useful in finding quantum generalizations of different inequalities in statistical mechanics of classical systems. Let us note that if the operator  $A$  commutes with the Hamiltonian  $\mathcal{H}$  (commutative case) the expressions (4) and (7) coincide. The genuine difference between (4) and (7) in the noncommutative case constitutes the novelty of the inequalities obtained below.

In the remainder we consider given observables  $A, B, C, \dots$  and fixed Hamiltonian  $\mathcal{H}$  pertaining to a quantum system in a finite region  $\Lambda$ . Whenever no confusion arises, for brevity of notation we will omit the subscripts  $\mathcal{H}$  and  $\Lambda$ , as well as the argument of the partition function  $Z$ .

## II. BOUNDS ON THE QUADRATIC FLUCTUATIONS

We assume that the Hamiltonian  $\mathcal{H}$  of the system in a finite region of space  $\Lambda$  is a self-adjoint, trace-class operator which generates the Gibbs semigroup  $\{\exp(-\beta\mathcal{H}_\Lambda)\}_{\beta \geq 0}$ . Let the operators  $A, B, \dots$ , belong to the algebra of bounded observables, for which the Bogoliubov - Duhamel inner product  $(A; B)$  is well defined.

Further we assume that the Hamiltonian  $\mathcal{H}$  has a discrete, non-degenerate spectrum only,  $\{E_n, n = 1, 2, 3, \dots\}$  and denote by  $|n\rangle$  the corresponding eigenfunctions, i.e.,  $\mathcal{H}|n\rangle = E_n|n\rangle$ ,  $n = 1, 2, 3, \dots$ . By  $A_{mn} = \langle m|A|n\rangle$  we denote the corresponding matrix element of an operator  $A$ . Then, the spectral representation of the Bogoliubov - Duhamel inner (6) can

be written as

$$(A; B)_{\mathcal{H}} = (Z_{\Lambda}[\mathcal{H}])^{-1} \sum'_{m,n} A_{mn}^* B_{mn} \frac{e^{-\beta E_m} - e^{-\beta E_n}}{\beta(E_n - E_m)} + (Z_{\Lambda}[\mathcal{H}])^{-1} \sum_n e^{-\beta E_n} A_{nn}^* B_{nn}, \quad (8)$$

where the prime in the double sum means that the term with  $n = m$  is excluded.

Our aim is to majorize the quadratic fluctuations

$$\langle \delta A^\dagger \delta A \rangle = \langle A^\dagger A \rangle_{\mathcal{H}} - |\langle A \rangle_{\mathcal{H}}|^2 \quad (9)$$

by terms proportional to some power of the inner product

$$\begin{aligned} (\delta A; \delta A) &= (A; A) - |\langle A \rangle|^2 \\ &= Z_{\Lambda}^{-1} \sum'_{m,n} |A_{mn}|^2 \frac{e^{-\beta E_m} - e^{-\beta E_n}}{\beta(E_n - E_m)} + (Z_{\Lambda}[\mathcal{H}])^{-1} \sum_n e^{-\beta E_n} |A_{nn}|^2 - |\langle A \rangle|^2. \end{aligned} \quad (10)$$

For the symmetrized form of (9) we obtain

$$\begin{aligned} &\frac{1}{2} \langle A^\dagger A + A A^\dagger \rangle - (A; A) \\ &= Z^{-1} \sum'_{m,n} |A_{mn}|^2 \left\{ \frac{1}{2} (e^{-\beta E_n} + e^{-\beta E_m}) - \frac{e^{-\beta E_m} - e^{-\beta E_n}}{\beta(E_n - E_m)} \right\}, \end{aligned} \quad (11)$$

which, by using the identity

$$e^{-\beta E_m} + e^{-\beta E_n} = (e^{-\beta E_n} - e^{-\beta E_m}) \coth \frac{\beta(E_m - E_n)}{2} \quad (12)$$

can be expressed as:

$$\frac{1}{2} \langle A^\dagger A + A A^\dagger \rangle - (A; A) = Z^{-1} \sum'_{m,n} |A_{mn}|^2 \frac{e^{-\beta E_m} - e^{-\beta E_n}}{\beta(E_n - E_m)} (X_{mn} \coth X_{mn} - 1), \quad (13)$$

where  $X_{mn} = \beta(E_m - E_n)/2$ .

Different choices of the upper bound on the right-hand side of (13) generate different inequalities. Thus, the inequality of Brooks Harris [8],

$$(A; A) \leq \frac{1}{2} \langle A A^\dagger + A^\dagger A \rangle \leq (A; A) + \frac{\beta}{12} \langle [[A^\dagger, \mathcal{H}], A] \rangle. \quad (14)$$

is obtained by setting  $1 \leq x \coth x \leq 1 + x^2/3$ .

On the other hand, if one uses another elementary inequality,  $1 \leq x \coth x \leq 1 + |x|$ , and subsequently applies the Hölder inequality, one obtains the result due to Ginibre [9]:

$$(A; A) \leq \frac{1}{2} \langle A A^\dagger + A^\dagger A \rangle \leq (A; A) + \frac{1}{2} \{ (A; A) \beta \langle [[A^\dagger, \mathcal{H}], A] \rangle \}^{\frac{1}{2}}. \quad (15)$$

A different choice of the parameters in the Hölder inequality, followed by the implementation of the upper bound

$$|e^{-\beta E_l} - e^{-\beta E_m}| < |e^{-\beta E_l} + e^{-\beta E_m}|, \quad (16)$$

generates a symmetric version of the inequality due to Bogoliubov Jr. [10]:

$$\frac{1}{2}\langle AA^+ + A^+A \rangle \leq (A; A) + \frac{1}{2}[(A; A)\beta]^{2/3}\{\langle [A^+, \mathcal{H}][\mathcal{H}, A] + [\mathcal{H}, A][A^+, \mathcal{H}] \rangle\}^{1/3}, \quad (17)$$

To derive generalizations of the known inequalities involving the Bogoliubov - Duhamel inner product, we define a set of new functionals in terms of their spectral representations:

$$\begin{aligned} F_{2n}(J; J) &\equiv Z^{-1} \sum_{ml} |J_{ml}|^2 |e^{-\beta E_l} - e^{-\beta E_m}| (\beta |E_m - E_l|)^{2n-1} \\ &= \beta^{2n} (R_n; R_n) = \beta^{2n-1} \langle [R_n^+ R_{n-1} - R_{n-1} R_n^+] \rangle, \quad n = 0, 1, 2, 3, \dots, \end{aligned} \quad (18)$$

where, by definition,  $R_{-1} \equiv X_{J\mathcal{H}}$  is a solution of the operator equation  $J = [X_{J\mathcal{H}}, \mathcal{H}]$ , and

$$R_0 \equiv R_0(J) = J, \quad R_1 \equiv R_1(J) = [\mathcal{H}, J], \quad \dots, \quad R_n \equiv R_n(J) = [\mathcal{H}, R_{n-1}(J)]. \quad (19)$$

The observables  $R_k$ ,  $k = 0, 1, 2, \dots$ , were introduced in [11]. Next, we have defined

$$\begin{aligned} F_{2n+1}(J; J) &\equiv Z^{-1} \sum_{ml} |J_{ml}|^2 (e^{-\beta E_l} + e^{-\beta E_m}) [\beta (E_m - E_l)]^{2n} \\ &= \beta^{2n} \langle [R_n R_n^+ + R_n^+ R_n] \rangle, \quad n = 0, 1, 2, 3, \dots \end{aligned} \quad (20)$$

In particular,

$$\begin{aligned} F_0(J; J) &= (J; J), \quad F_1(J; J) = \langle J J^+ + J^+ J \rangle, \quad F_2(J; J) = \beta \langle [J^+, \mathcal{H}], J \rangle, \\ F_3(J; J) &= \beta^2 \langle [J^+, \mathcal{H}][\mathcal{H}, J] + [\mathcal{H}, J][J^+, \mathcal{H}] \rangle. \end{aligned} \quad (21)$$

The functionals (18) and (20) are used to generalize all the known inequalities used in the Approximating Hamiltonian method. Here we give the final results:

### A. The generalized Harris inequality

For all integers  $n = 0, 1, 2, \dots$  we have

$$F_{2n}(J; J) \leq \frac{1}{2} F_{2n+1}(J; J) \leq F_{2n}(J; J) + \frac{1}{12} F_{2n+2}(J; J). \quad (22)$$

The Brooks Harris inequality (14) is recovered when  $n = 0$ .

### B. The generalized Plechko inequalities

The following inequalities were proved to hold for all  $p, q > 1$ , such that  $1/p + 1/q = 1$ :

$$\begin{aligned} & (2Z)^{-1} \sum_{ml} |J_{ml}|^2 |e^{-\beta E_l} - e^{-\beta E_m}| [\beta(E_m - E_l)]^{2n} \\ & \leq \frac{1}{2} (J; J)^{1/p} \left\{ Z^{-1} \sum_{ml} |J_{ml}|^2 \frac{e^{-\beta E_l} - e^{-\beta E_m}}{\beta(E_m - E_l)} [\beta(E_m - E_l)]^{(2n+1)q} \right\}^{1/q}. \end{aligned} \quad (23)$$

One of the possible choices of  $p$  and  $q$  here is even integer  $q = 2k$  (hence,  $p = 2k/(2k-1)$ ) which leads to the set of generalized Ginibre inequalities.

### C. The generalized Ginibre inequalities

These inequalities read ( $k = 1, 2, 3, \dots$ ):

$$F_{2n}(J; J) \leq \frac{1}{2} F_{2n+1}(J; J) \leq F_{2n}(J; J) + \frac{1}{2} (J; J)^{(2k-1)/2k} [F_{2k(2n+1)}(J; J)]^{1/2k}. \quad (24)$$

At  $n = 0$  the above set reduces to a symmetric version of the inequalities obtained by Plechko [12]:

$$(J; J) \leq \frac{1}{2} \langle J J^+ + J^+ J \rangle \leq (J; J) + \frac{1}{2} (J; J)^{(2k-1)/2k} \beta(R_k; R_k)^{1/2k}, \quad (k = 1, 2, 3, \dots). \quad (25)$$

Hence, in the particular case of  $k = 1$  one obtains the Ginibre inequality (15).

### D. The generalized Bogoliubov Jr. - Plechko - Repnikov inequalities

These inequalities are obtained from (23) under the choice of odd  $q = 2k + 1$ , hence,  $p = (2k + 1)/2k$ ,  $k = 1, 2, 3, \dots$ :

$$\frac{1}{2} F_{2n+1}(J; J) \leq F_{2n}(J; J) + \frac{1}{2} (J; J)^{2k/(2k+1)} [F_{2(2nk+n+k)+1}(J; J)]^{1/(2k+1)}. \quad (26)$$

At  $n = 0$  these reduce to a symmetric version of the set of inequalities obtained by Bogoliubov Jr., Plechko and Repnikov [11]:

$$\frac{1}{2} \langle J J^+ + J^+ J \rangle \leq (J; J) + \frac{1}{2} (J; J)^{2k/(2k+1)} \{ \beta^{2k} \langle R_k R_k^+ + R_k^+ R_k \rangle \}^{1/(2k+1)}. \quad (27)$$

The symmetric version of the inequality due to Bogoliubov Jr. (17) follows from here in the particular case of  $k = 1$ .

In [7] we have shown that under sufficiently mild conditions, each of the generalized upper bounds has the same form and order of magnitude with respect to the number of particles (or volume) for all the quantities derived by commutations of an intensive observable with the Hamiltonian of the system. An application of the generalized inequalities to a quantum spin model with separable attraction and the Dicke model of superradiance was given too.

### III. FIDELITY SUSCEPTIBILITY AND GIBBS THERMAL STATES

Over the last decade there have been impressive theoretical advances concerning the concepts of entanglement and fidelity from quantum and information theory [13],[14], and their application in condensed matter physics, especially in the theory of critical phenomena and phase transitions, for a review see [5, 15]. These two concepts are closely related to each other.

The fidelity [16, 17] naturally appears in quantum mechanics as the absolute value of the overlap (Hilbert-space scalar product) of two quantum states corresponding to different values of the control parameters. The corresponding finite-temperature extension, defined as a functional of two density matrices,  $\rho_1$  and  $\rho_2$ ,

$$\mathcal{F}(\rho_1, \rho_2) = \text{Tr} \sqrt{\rho_1^{1/2} \rho_2 \rho_1^{1/2}}, \quad (28)$$

was introduced by Uhlmann [18] and called fidelity by Jozsa [16].

Being a measure of the similarity between quantum states, both pure or mixed, fidelity should decrease abruptly at a critical point, thus locating and characterizing the phase transition. Different finite-size scaling behaviors of the fidelity indicate different types of phase transitions. The fidelity approach is basically a metric one and has an advantage over the traditional Landau-Ginzburg theory, because it avoids possible difficulties in identifying the notions of order parameter, symmetry breaking, correlation length and so it is suitable for the study of different kinds of topological or Berezinskii-Kosterlitz-Thouless phase transitions.

The above mentioned decrease in the fidelity  $\mathcal{F}(\rho_1, \rho_2)$ , when the state  $\rho_2$  approaches a quantum critical state  $\rho_1$ , is associated with a divergence of the fidelity susceptibility  $\chi_F(\rho_1)$  which reflects the singularity of  $\mathcal{F}(\rho_1, \rho_2)$  at that point. The fidelity susceptibility  $\chi_F(\rho_1)$ , which is the main objects of this study, naturally arises as a leading-order term in the expansion of the fidelity for two infinitesimally close density matrices  $\rho_1$  and  $\rho_2 =$

$\rho_1 + \delta\rho$ . For simplicity, in this section and thorough the rest of the paper we set in (1)  $|\Lambda|(\nu A^\dagger + \nu^* A) = hS$ , where  $h = \nu = \nu^*$  is a real parameter. Following our study [6], we consider the one-parameter family of Gibbs states

$$\rho(h) = [Z(h)]^{-1} \exp[-\beta T + \beta h S], \quad (29)$$

defined on the family of Hamiltonians of the form  $H(h) = T - hS$ , where the Hermitian operators  $T$  and  $S$  do not commute in the general case,  $h$  is a real parameter, and  $Z(h) = \text{Tr} \exp[-\beta T + \beta h S]$  is the corresponding partition function. There are two natural definitions of the fidelity susceptibility at the point  $h = 0$ , depending on the type of approach to that point:

(i) The one-sided fidelity susceptibility at the point  $h = 0$  in the parameter space is defined as (see e.g. [19]):

$$\chi_F(\rho(0)) := \lim_{h \rightarrow 0} \frac{-2 \ln \mathcal{F}(\rho(0), \rho(h))}{h^2} = - \left. \frac{\partial^2 \mathcal{F}(\rho(0), \rho(h))}{\partial h^2} \right|_{h=0}. \quad (30)$$

Starting from this definition, in our work [6] we derived a spectral representation for  $\chi_F(\rho(0))$  which was used to obtain lower and upper bounds on the fidelity susceptibility.

(ii) One may consider also a symmetric two-sided definition of the fidelity susceptibility at the point  $h = x \in R$ , given by

$$\chi_F^{(2)}(\rho(x)) := \lim_{h \rightarrow 0} \frac{-2 \ln \mathcal{F}(\rho(x - h/2), \rho(x + h/2))}{h^2} = - \left. \frac{\partial^2 \mathcal{F}(\rho(x - h/2), \rho(x + h/2))}{\partial h^2} \right|_{h=0}. \quad (31)$$

To avoid confusion, we point out that for mixed states the definition of the fidelity susceptibility (30), based on the Uhlmann fidelity (28), differs from the one derived in [20] (see also [5]) by extending the ground-state Green's function representation to nonzero temperatures, even both have the same  $T = 0$  limit. This fact has been pointed out in [21], see also our discussion in [6]. Along with the statistical mechanical notion of susceptibility, the quantity (30) is known also as “Bures metric over the thermal states” [20, 22], thus introducing the geometric approach in the field.

To proceed with the calculations when the operators  $T$  and  $S$  do not commute, one has to consider a convenient spectral representation. To simplify the problem, we assume that the Hermitian operator  $T$  has a complete orthonormal set of eigenvectors  $|n\rangle$ ,  $T|n\rangle = T_n|n\rangle$ , where  $n = 1, 2, \dots$ , with non-degenerate spectrum  $\{T_n\}$ .



In the one-sided case (30), the following spectral representation was obtained [6]:

$$\begin{aligned}\chi_F(\rho) &= \frac{1}{2} \sum_{m,n} \frac{|\langle m|\rho'(0)|n\rangle|^2}{\rho_m + \rho_n} \\ &= \frac{\beta^2}{8} \sum_{m,n,m \neq n} \frac{\rho_n - \rho_m}{X_{mn}} \frac{|\langle n|S|m\rangle|^2}{X_{mn} \coth X_{mn}} + \frac{1}{4} \beta^2 \langle (\delta S^d)^2 \rangle_0.\end{aligned}\quad (32)$$

Here  $X_{mn} \equiv \beta(T_m - T_n)/2$ ,  $\langle \cdots \rangle_0$  denotes the Gibbs average value at  $h = 0$ ,  $\delta S^d = S^d - \langle S^d \rangle_0$ , where  $S^d$  is the diagonal part of the operator  $S$ , so that

$$\langle (\delta S^d)^2 \rangle_0 := \sum_m \rho_m \langle m|S|m\rangle^2 - \langle S \rangle_0^2. \quad (33)$$

Representation (32) was the starting point for the derivation of inequalities involving macroscopic quantities, like susceptibilities and thermal average values. Note that the first term in the right-hand side describes the purely quantum contribution to the fidelity susceptibility, which vanishes when the operators  $T$  and  $S$  commute, while the second term represents the “classical” contribution.

By comparing definitions (30) and (31) in the non-commutative case, one sees an essential difference: in the one-sided case the zero-field density matrix  $\rho(0)$  is diagonal in the basis spanned by the eigenfunctions of the operator  $T$ ,  $\langle m|\rho(0)|n\rangle = \rho_m(0)\delta_{m,n}$ ,  $m, n = 1, 2, \dots$ , while in the two-sided case (31) both  $\rho(-h/2)$  and  $\rho(h/2)$  have non-diagonal elements. Hence, it is not obvious that the two-sided fidelity susceptibility will have the same spectral representation (32) and, the following from it, lower and upper bounds. This observation has motivated us to give an independent derivation of the spectral representation for  $\chi_F^{(2)}(\rho(0))$ .

#### IV. DERIVATION OF THE SPECTRAL REPRESENTATION FOR THE SYMMETRIC TWO-SIDED FIDELITY SUSCEPTIBILITY

For the family of density matrices of the form (29) we consider the slightly more general case of a two-sided fidelity around a point  $x \in R$ :

$$\mathcal{F}(\rho(x-y), \rho(x+y)) = \text{Tr} \sqrt{\rho^{1/2}(x-y) \rho(x+y) \rho^{1/2}(x-y)}, \quad y \in R. \quad (34)$$

Assume that  $\{|n\rangle, n = 1, 2, \dots\}$  is a complete set of eigenvectors of the Hamiltonian  $H(x) = T - xS$ , with eigenvalues  $E_n(x)$ :  $(T - xS)|n\rangle = E_n(x)|n\rangle$ . In this basis the density matrix  $\rho(x)$  is diagonal too, which implies  $\langle m|\rho(x)|n\rangle = \rho_n(x)\delta_{m,n}$ , for all  $m, n = 1, 2, \dots$ .

In order to calculate the symmetric two-sided fidelity susceptibility at  $y = 0$ , we need the  $O(h^2)$  term in the expansion of (34) in powers of  $h \rightarrow 0$ . Consider first the expansions

$$\rho(x \pm y) = \rho(x) \pm y\rho'(x) + \frac{1}{2}y^2\rho''(x) + r_{\pm}, \quad (35)$$

where  $r_{\pm}$  are bounded operators of the order  $O(h^3)$ . From the normalization condition for the density matrices,  $\text{Tr}\rho(x \pm y) = \text{Tr}\rho(x) = 1$ , it follows that

$$\text{Tr}\rho'(x) = \text{Tr}\rho''(x) = 0. \quad (36)$$

To calculate the square root of  $\rho(x - y)$  up to the order  $O(h^2)$ , we set

$$\rho^{1/2}(x \pm y) = \rho^{1/2}(x) \pm A + B + C_{\pm}, \quad (37)$$

where  $A$ ,  $B$ , and  $C_{\pm}$  are bounded operators of the order of  $y$ ,  $y^2$ , and  $y^3$ , respectively. Then, by comparing the squared of (37) with the expansion (35) for  $\rho(x - y)$ , we obtain

$$\begin{aligned} y\rho'(x) &= \rho^{1/2}(x)A + A\rho^{1/2}(x), \\ \frac{1}{2}y^2\rho''(x) &= A^2 + \rho^{1/2}(x)B + B\rho^{1/2}(x). \end{aligned} \quad (38)$$

Hence, we find the matrix elements of the operators  $A$  and  $B$ :

$$\langle m|A|n \rangle = y \frac{\langle m|\rho'(x)|n \rangle}{\rho_m^{1/2}(x) + \rho_n^{1/2}(x)}, \quad (39)$$

$$\langle m|B|n \rangle = -\frac{\langle m|A^2|n \rangle}{\rho_m^{1/2}(x) + \rho_n^{1/2}(x)} + \frac{1}{2}y^2 \frac{\langle m|\rho''(x)|n \rangle}{\rho_m^{1/2}(x) + \rho_n^{1/2}(x)}. \quad (40)$$

Next, with the aid of expansions (35) and (37) we evaluate, up to order  $O(y^2)$ , the product

$$\begin{aligned} \rho^{1/2}(x - y)\rho(x + y)\rho^{1/2}(x - y) &= \rho^2(x) - A\rho^{3/2}(x) - \rho^{3/2}(x)A + y\rho^{1/2}(x)\rho'(x)\rho^{1/2}(x) \\ &+ A\rho(x)A - yA\rho'(x)\rho^{1/2}(x) - y\rho^{1/2}(x)\rho'(x)A + \frac{1}{2}y^2\rho^{1/2}(x)\rho'(x)\rho^{1/2}(x) \\ &+ B\rho^{3/2}(x) + \rho^{3/2}(x)B + O(y^3). \end{aligned} \quad (41)$$

Next, following the standard scheme proposed in [23], we set

$$\sqrt{\rho^{1/2}(x - y)\rho(x + y)\rho^{1/2}(x - y)} = \rho(x) + X + Y + Z, \quad (42)$$

where  $X$ ,  $Y$ , and  $Z$  are bounded operators of the order of  $y$ ,  $y^2$ , and  $y^3$ , respectively, and compare the terms of the same order of magnitude in the right-hand sides of (41) and the squared of (42). Within the order  $O(y)$  we obtain

$$\rho(x)X + X\rho(x) = -A\rho^{3/2}(x) - \rho^{3/2}(x)A + y\rho^{1/2}(x)\rho'(x)\rho^{1/2}(x) \quad (43)$$

By taking matrix elements with the eigenvectors of  $H(x)$  and using expression (39) for  $\langle m|A|n\rangle$ , we find

$$\begin{aligned} & [\rho_m(x) + \rho_n(x)]\langle m|X|n\rangle = \\ & -y \frac{\langle m|\rho'(x)|n\rangle}{\rho_m^{1/2}(x) + \rho_n^{1/2}(x)} [\rho_m^{3/2}(x) + \rho_n^{3/2}(x)] + y\rho_m^{1/2}(x)\rho_n^{1/2}(x)\langle m|\rho'(x)|n\rangle = \\ & -y\langle m|\rho'(x)|n\rangle[\rho_m^{1/2}(x) - \rho_n^{1/2}(x)]^2. \end{aligned} \quad (44)$$

Therefore,

$$\langle m|X|n\rangle = -y \frac{\langle m|\rho'(x)|n\rangle}{\rho_m(x) + \rho_n(x)} [\rho_m^{1/2}(x) - \rho_n^{1/2}(x)]^2. \quad (45)$$

One important consequence of this equality is the vanishing of the diagonal elements of  $X$ , hence  $\text{Tr}X = 0$ .

Next, within the order  $O(y^2)$ , from (41) and the square of expression (42) we obtain

$$\begin{aligned} X^2 + \rho(x)Y + Y\rho(x) &= A\rho(x)A - yA\rho'(x)\rho^{1/2}(x) - y\rho^{1/2}(x)\rho'(x)A \\ &+ \frac{1}{2}y^2\rho^{1/2}(x)\rho''(x)\rho^{1/2}(x) + B\rho^{3/2}(x) + \rho^{3/2}(x)B. \end{aligned} \quad (46)$$

For our needs it suffices to take the diagonal elements of the above equality

$$\begin{aligned} \langle n|X^2|n\rangle + 2\rho_n(x)\langle n|Y|n\rangle &= \langle n|A\rho(x)A|n\rangle - y\rho_n^{1/2}(x)\langle n|A\rho'(x) + \rho'(x)A|n\rangle \\ &+ \frac{1}{2}y^2\rho_n(x)\langle n|\rho''(x)|n\rangle + 2\rho_n^{3/2}(x)\langle n|B|n\rangle, \end{aligned} \quad (47)$$

and evaluate  $\text{Tr}Y$ . Since the calculations are rather involved, we present them in some detail. Taking into account Eqs. (39), (40) and (45), we obtain the expression

$$\begin{aligned} \text{Tr}Y &\equiv \sum_n \langle n|Y|n\rangle = -\frac{1}{2}y^2 \sum_{m,n} |\langle n|\rho'(x)|m\rangle|^2 \frac{[\rho_m^{1/2}(x) - \rho_n^{1/2}(x)]^4}{\rho_n(x)[\rho_m(x) + \rho_n(x)]^2} \\ &+ \frac{1}{2}y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2 \rho_m(x)}{\rho_n(x)[\rho_m^{1/2}(x) + \rho_n^{1/2}(x)]^2} - y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2}{\rho_n^{1/2}(x)[\rho_m^{1/2}(x) + \rho_n^{1/2}(x)]} \\ &+ \frac{1}{2}y^2 \text{Tr}\rho''(x) - \frac{1}{2}y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2}{[\rho_m^{1/2}(x) + \rho_n^{1/2}(x)]^2}. \end{aligned} \quad (48)$$

Now we note that the forth term in the right-hand side of the above equality is zero due to (36). The sum of the second and fifth terms yields

$$\frac{1}{2}y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2 [\rho_m(x) - \rho_n(x)]}{\rho_n(x)[\rho_m^{1/2}(x) + \rho_n^{1/2}(x)]^2} = \frac{1}{2}y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2 [\rho_m^{1/2}(x) - \rho_n^{1/2}(x)]}{\rho_n(x)[\rho_m^{1/2}(x) + \rho_n^{1/2}(x)]}. \quad (49)$$

Next, by writing  $[\rho_m^{1/2} - \rho_n^{1/2}]^4 = (\rho_m + \rho_n)^2 - 4\rho_m^{1/2}\rho_n^{1/2}(\rho_m + \rho_n) + 4\rho_m\rho_n$ , we split the first sum in the right-hand side of (48) into a sum of three terms:

$$-\frac{1}{2}y^2 \sum_{m,n} |\langle n|\rho'(x)|m\rangle|^2 \left[ \frac{1}{\rho_n(x)} - \frac{4\rho_m^{1/2}(x)}{\rho_n^{1/2}(x)[\rho_m(x) + \rho_n(x)]} + \frac{4\rho_m(x)}{[\rho_m(x) - \rho_n(x)]^2} \right]. \quad (50)$$

By adding up (49) with the third term in (48) and the first term coming from (50) we obtain

$$-2y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2}{\rho_n^{1/2}(x)[\rho_m^{1/2}(x) + \rho_n^{1/2}(x)]}. \quad (51)$$

Remarkably, the sum of the above result with the second term coming from (50) vanishes:

$$2y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2 [\rho_m^{1/2}(x) - \rho_n^{1/2}(x)]}{[\rho_m^{1/2}(x) + \rho_n^{1/2}(x)][\rho_m(x) + \rho_n(x)]} = 0. \quad (52)$$

Therefore, we are left with the contribution of the last term in (50), hence

$$\text{Tr}Y = -2y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2 \rho_m(x)}{[\rho_m(x) + \rho_n(x)]^2} = -y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2}{[\rho_m(x) + \rho_n(x)]}. \quad (53)$$

Thus, taking trace of both sides of equality (42), we obtain the two-sided symmetric fidelity (34) up to the order  $O(y^2)$ :

$$\mathcal{F}(\rho(x-y), \rho(x+y)) = 1 - y^2 \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2}{[\rho_m(x) + \rho_n(x)]}, \quad x, y \in R. \quad (54)$$

Hence, by setting here  $y = h/2$ , from the definition (31) of the fidelity susceptibility, it follows that

$$\chi_F^{(2)}(\rho(x)) = \frac{1}{2} \sum_{m,n} \frac{|\langle n|\rho'(x)|m\rangle|^2}{[\rho_m(x) + \rho_n(x)]}. \quad (55)$$

At  $x = 0$  this expression reduces exactly to the spectral representation (32) found in our work [6] for the zero-field one-sided fidelity susceptibility.

## V. LOWER AND UPPER BOUNDS ON THE FIDELITY SUSCEPTIBILITY

Bounds on the fidelity susceptibility follow by applying elementary inequalities for  $(x \coth x)^{-1}$  to the summand in expression (32). In our paper [6] an upper bound on  $\chi_F(\rho)$  was obtained in the transparent form

$$\chi_F(\rho) \leq \frac{\beta^2}{4} (\delta S; \delta S)_0, \quad (56)$$

where  $(\delta S; \delta S)_0$  is the Bogoliubov-Duhamel inner product of the self-adjoint operator  $\delta S$  with itself in the Gibbs ensemble with Hamiltonian  $H(0) = T$ . Note that the right-hand side of the above inequality is proportional to the initial thermodynamic susceptibility:

$$(\delta S; \delta S)_0 = -\frac{N}{\beta} \frac{\partial^2 f[H(h)]}{\partial^2 h} \Big|_{h=0} = \frac{N}{\beta} \chi_N, \quad (57)$$

where  $f[H(h)]$  is the free energy density of the system described by the Hamiltonian  $H(h)$  and  $\chi_N$  is the susceptibility with respect to the field  $h$ .

On the other hand, by applying to the spectral representation for the fidelity susceptibility (32) the elementary inequality  $(x \coth x)^{-1} \geq 1 - (1/3)x^2$ , we have obtained the following lower bound

$$\chi_F(\rho) \geq \frac{\beta^2}{4} (\delta S; \delta S)_0 - \frac{\beta^3}{48} \langle [[S, T], S] \rangle_0. \quad (58)$$

The quality of the derived upper and lower bounds was tested in the simplest case of a single spin in external magnetic field, subject to a transverse-field perturbation. Finally, these bounds were applied to two many-body quantum-mechanical models: the single impurity Kondo model and the Dicke model of superradiance. In conclusion, our lower (58) and upper (56) bounds indicate that for the detection of a second order phase transition, with diverging in the thermodynamic limit susceptibility, the fidelity susceptibility per particle  $\chi_F/N$  is as efficient as the usual susceptibility  $\chi$ . This conclusion is in conformity with the commonly accepted view that quantum fluctuations are dominated by the thermal ones when  $T_c > 0$ . However, one should keep in mind that our results were derived under rather restrictive conditions on the spectrum of the Hamiltonian.

## VI. CONCLUDING REMARKS

The infinite sets of generalized statistical mechanical inequalities presented in Section II provide upper bounds on the difference between the quadratic fluctuations of intensive observables expressed in terms of the corresponding Bogoliubov - Duhamel inner product and Gibbs average values of their commutator with the Hamiltonian. Such bounds are used, e.g., in the majorization technique developed by Bogoliubov Jr. for the needs of the Approximating Hamiltonian method [10]. A survey of inequalities used to solve problems arising in the Approximating Hamiltonian Method, along with their generalizations, is given in our paper [7]. The results are illustrated by two types of exactly solvable model systems:

one with bounded separable attraction and the other describing interaction of a boson field with matter.

In Section III, some subtle points in the definition of the thermal fidelity susceptibility are discussed. The concept of fidelity susceptibility naturally appears as the fidelity's leading term in the perturbation expansion with respect to the infinitesimal deviation from a particular point of the parameter space. So it is possible to have different definitions depending on the way this point is approached. Two definitions are commonly considered: a one-sided second derivative with respect of the parameter distinguishing the two density matrices, or a symmetric two-sided derivative. In the next Section IV, it is shown that the final result for the spectral presentation of the fidelity susceptibility does not depend on which of the two definitions is used. While it seems intuitively reasonable, it is nevertheless important to prove this statement.

In Section V, we have presented bounds on the fidelity susceptibility, a notion from the information theory, which are expressed in terms of quantities from the statistical mechanics, thus emphasizing connection points between these two disciplines. An additional reason that stimulates this line of consideration of information-theoretic quantities is that the experimental setup for measuring thermodynamic quantities is well developed. Thus, estimation of metric quantities with the aid of thermodynamic-based experiments seems to be very appealing. Note that the fidelity susceptibility reduces down to the Fisher information (for details see, e. g., [22, 24] and references therein) which provides another line of applicability of our results to quantum estimation theory.

We have shown that as far as divergent behavior in the thermodynamic limit is considered, the fidelity susceptibility  $\chi_F$  and the usual thermodynamic susceptibility  $\chi$  are equivalent for a large class of models exhibiting critical behavior. It remains for the future to study the effect of the degeneracy of the ground state, especially of a macroscopic one, on the upper and lower bounds for the fidelity susceptibility.

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